Supporting Information

Chiral Aromatase and Dual Aromatase-Steroid Sulfatase Inhibitors from the Letrozole Template: Synthesis, Absolute Configuration and In Vitro Activity

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Contents:

Experimental procedures

General Method A – Condensation of carbinols with triazole. The substrate, 1,2,4-triazole and *para*-toluenesulfonic acid (*p*-TSA), dissolved/suspended in toluene were heated at reflux with a Dean-Stark separator for 24 h. The reaction mixture was allowed to cool, and the solvent was removed *in vacuo.*

2-Benzyloxy-4-bromo-1-methoxybenzene (12). NaH (60% in mineral oil, 0.61 g, 15.3 mmol) was added in three equal portions to a cooled (0 °C) solution of 5-bromo-2-methoxyphenol[1] **11** (2.60 g, 12.8 mmol) in DMF (25 mL). After 20 minutes, benzyl bromide (2.63 g, 15.3 mmol) was added and the reaction mixture was allowed to warm to room temperature and was stirred overnight. The reaction mixture was poured onto H_2O (100 mL) and extracted with EtOAc (4 x 50 mL). The combined organic layers were washed with H_2O (4 x 75 mL) and brine (75 mL), dried ($MgSO_4$) and the solvent was removed *in vacuo*. The crude product was purified by recrystallization from Et_2O to give the title compound (2.90 g, 77%, mp 109-110 °C [lit. 105-106 °C (Et_2O)[2]]) as a white crystalline solid; δ_H (270 MHz, $CDCl_3$) 7.47-7.26 (5H, m, Ar*H*), 7.07-7.00 (2H, m, Ar*H*), 6.74 (1H, d, *J*=8.7, Ar*H*), 5.10 (2H, s, CH_2), 3.85 (3H, s, CH_3).

1-Benzyloxy-4-bromo-2-methoxybenzene (18). NaH (60% in mineral oil, 0.95 g, 23.6 mmol) was added in three equal portions to a cooled (0 °C) solution of 4-bromoguaiacol (**17**) (4.0 g, 19.7 mmol) in DMF (40 mL). After 20 minutes, benzyl bromide (4.04 g, 23.6 mmol) was added and the reaction mixture was allowed to warm to room temperature and was stirred overnight. The reaction mixture was poured onto H_2O (60 mL) and extracted with EtOAc (4 x 60 mL). The combined organic layers were washed with H_2O (3 x 70 mL) and brine (70 mL), dried ($MgSO_4$) and the solvent was removed *in vacuo*. The crude product was purified by recrystallization from EtOH to give the title compound (4.57 g, 79%, mp 59-61 °C [lit. 61-61.2 °C (EtOH)[3]]) as a white crystalline solid; δ_H (270 MHz, $CDCl_3$) 7.47-7.24 (5H, m, Ar*H*), 7.03-6.91 (2H, m, Ar*H*), 6.73 (1H, d, *J*=8.4, Ar*H*), 5.11 (2H, s, CH_2), 3.86 (3H, s, CH_3).

***Bis*-(4-benzyloxy-3-methoxyphenyl)methanol (19).** *n*-BuLi (1.3 M, 8.7 mL) was added slowly to a cooled (-78 °C) solution of **18** (3.00 g, 10.24 mmol) in THF (40 mL). After stirring for 1 h, a solution of 4-benzyloxy-3-methoxy-benzaldehyde (2.48 g, 10.24 mmol) in THF (24 mL) was added dropwise and the reaction mixture was stirred for 1.5 h. The reaction mixture was allowed to warm to room temperature and after stirring for 2 h it was quenched by the addition of H_2O (150 mL). The product was extracted with EtOAc (3 x 150 mL) and the combined organics were dried ($MgSO_4$), and the solvent was removed *in vacuo*. The crude product was purified by precipitation from EtOAc/hexane to give the title compound (3.03 g, 65%, mp 102-103 °C) as a white solid; δ_H (270 MHz, $CDCl_3$) 7.49-7.21 (10H, m, Ar*H*), 6.92 (2H, d, *J*=1.5, ArH), 6.84-6.72 (4H, m, Ar*H*), 5.70 (1H, d, *J*=3.2, C*H*), 5.13 (4H, s, 2 x CH_2), 3.84 (6H, s, 2 x CH_3), 2.20 (1H, d, *J*=3.2, O*H*); δ_C (100 MHz, DMSO-d_6) 149.7 (2 x C), 147.7 (2 x C), 137.3 (2 x C), 137.2 (2 x C), 128.7 (4 x CH), 128.0 (2 x CH), 127.4 (4 x CH), 119.0 (2 x CH), 113.8 (2 x CH), 110.4 (2 x CH), 76.0 (CH), 71.2 (2 x CH_2), 56.3 (2 x CH_3); LRMS (FAB^+) 456.2 (M^+, 50%), 439.2 (70), 243.2 (20), 91.1 (100); HRMS (FAB^+) Found 479.1819, $C_{29}H_{28}NaO_5$ $[M+Na]^+$ requires 479.1829.

1-[*Bis*-(4-benzyloxy-3-methoxyphenyl)methyl]-1*H*-[1,2,4]triazole (20). As general method A using **19** (2.30 g, 5.04 mmol), 1,2,4-triazole (0.70 g, 10.08 mmol), *p*-TSA (230 mg) and toluene (250 mL). The resulting residue was dissolved in EtOAc (100 mL) and H_2O (100 mL) and the layers were separated. The organic layer was washed with H_2O (2 x 100 mL), dried ($MgSO_4$) and the solvent was removed *in vacuo*. The crude product was purified using Flashmaster II (EtOAc/Hexane) to give the title compound (2.21 g, 86%, mp 107-108.5 °C) as a yellow oil which solidified after standing; δ_H (270 MHz, $CDCl_3$) 8.00 (1H, s, NC*H*N), 7.89 (1H, s, NC*H*N), 7.46-7.24 (10H, m, Ar*H*), 6.84 (2H, d, *J*=8.4, Ar*H*), 6.66 (2H, d, *J*=2.2, Ar*H*), 6.61 (1H, s, Ar*H*), 6.53 (2H, dd, *J*=8.4, 2.2, Ar*H*), 5.13 (4H, s, 2 x CH_2), 3.76 (6H, s, 2 x CH_3); δ_C (100 MHz, $CDCl_3$) 152.4 (CH), 150.0 (2 x C), 148.4 (2 x C), 143.6 (CH), 136.9 (2 x C), 131.0 (2 x C), 128.8 (4 x CH), 128.2 (2 x CH), 127.4 (4 x CH), 120.6 (2 x CH), 113.9 (2 x CH), 111.8 (2 x CH), 71.3 (2 x CH_2), 67.7 (CH), 56.4 (2 x CH_3); LRMS (FAB^+) 507.1 (M^+,

35%), 439.1 (100), 349.1 (15), 257.1 (10), 91.1 (100); HRMS (FAB^+) Found 507.2150, $C_{31}H_{29}N_3O_4$ requires 507.2158.

4-Cyano-4'-hydroxybenzophenone (25). A mixture of 4-cyano-4'-methoxybenzophenone[4] **24** (0.75 g, 3.16 mmol) and pyridine hydrochloride (3.66 g, 31.7 mmol) were slowly heated together to 210 °C with stirring and then maintained at this temperature for 20 min. The resulting dark brown solution was poured whilst still hot onto H_2O (75 mL) and the precipitate was collected by filtration and purified using Flashmaster II (EtOAc/Hexane). The title compound (0.42 g, 60%, mp 192.5-194 °C [lit. 186-189 °C[5]]) was obtained as a white powder; δ_H (270 MHz, DMSO-d_6), 10.60 (1H, br s, O*H*) 8.01 (2H, AA'BB', Ar*H*), 7.81 (2H, AA'BB', Ar*H*), 7.69 (2H, AA'BB', Ar*H*), 6.91 (2H, AA'BB', Ar*H*).

(4-Cyanophenyl)(4-hydroxyphenyl)methanol (26). A solution of $NaBH_4$ (0.37 g, 9.79 mmol) in H_2O (10 mL) was added dropwise to a solution of **25** (2.00 g, 8.96 mmol) in EtOH (30 mL). After stirring for 5 h, the reaction mixture was added to aq. HCl (1.5 M, 50 mL) and the product was extracted with EtOAc (3 x 50 mL). The combined organic layers were washed with brine (150 mL), dried ($MgSO_4$) and the solvent was removed *in vacuo*. The crude product was purified using Flashmaster II (EtOAc/Hexane) to give the title compound (1.49 g, 74%, mp 159-161 °C) as a white solid; δ_H (400 MHz, DMSO-d_6), 9.31 (1H, br s, O*H*) 7.73 (2H, AA'BB', Ar*H*), 7.51 (2H, AA'BB', Ar*H*), 7.11 (2H, AA'BB', Ar*H*), 6.66 (2H, AA'BB', Ar*H*), 5.96 (1H, br s, O*H*), 5.66 (1H, s, C*H*); δ_C (100 MHz, DMSO-d_6) 157.0 (C), 152.2 (C), 135.7 (C), 132.7 (2 x CH), 128.3 (2 x CH), 127.5 (2 x CH), 119.8 (C), 115.6 (2 x CH), 109.8 (C), 74.1 (CH); Anal. ($C_{14}H_{11}NO_2$) C, H, N.

4-Cyano-3'-chloro-4'-methoxybenzophenone (30). Aluminium chloride (5.31 g, 39.8 mmol) was added in small portions over 15 minutes to a solution of 4-cyanobenzoyl chloride (6.00 g, 36.2 mmol) in *o*-chloroanisole (**29**) (30 mL). After stirring for 24h, the reaction mixture was poured onto ice-water (80 mL) and stirred for 1 h. EtOAc (80 mL) and 3M NaOH (50 mL) were added and the layers were separated; the aqueous was further extracted with EtOAc (2 x 80 mL). The organic layers were combined, washed with brine (2 x 100 mL) and then dried ($MgSO_4$). The solvent was removed *in*

vacuo to give a dark brown oil to which hexane (200 mL) was added. The white precipitate was collected and was purified by two recrystallizations from EtOH to give the title compound (3.74 g, 38%, mp 169-170.5 °C) as a white crystalline solid; δ_H (270 MHz, DMSO-d_6), 8.03 (2H, AA'BB', Ar*H*), 7.84 (2H, AA'BB', Ar*H*), 7.81 (1H, d, *J*=2.1, Ar*H*), 7.72 (1H, dd, *J*=8.6, 2.1, Ar*H*), 7.32 (1H, d, *J*=8.6, Ar*H*), 3.98 (3H, s, CH_3); δ_C (100 MHz, DMSO-d_6) 192.9 (C), 159.0 (C), 141.6 (C), 133.1 (2 x CH), 131.8 (CH), 131.7 (CH), 130.3 (2 x CH), 129.7 (C), 122.1 (C), 118.7 (C), 114.8 (C), 113.0 (CH), 57.2 (CH_3); LCMS (APCI$^-$) 271.0 (M^-, 5%), 255.9 (70); HRMS (FAB$^+$) Found 272.0476, $C_{15}H_{11}NO_2Cl$ requires 272.0478.

4-Cyano-3'-chloro-4'-hydroxybenzophenone (31). A mixture of **30** (3.00 g, 11.0 mmol) and pyridine hydrochloride (12.76 g, 0.11 mol) were heated together slowly to 210 °C with stirring and then maintained at this temperature for 20 min. The resulting dark brown solution was poured whilst still hot onto H_2O (250 mL) and the precipitate was collected by filtration and purified using Flashmaster II (EtOAc/Hexane). The title compound (2.54 g, 91%, mp 206.5-208.5 °C) was obtained as a white solid; δ_H (270 MHz, DMSO-d_6), 11.46 (1H, br s, O*H*), 8.04 (2H, AA'BB', Ar*H*), 7.83 (2H, AA'BB', Ar*H*), 7.76 (1H, d, *J*=2.0, Ar*H*), 7.61 (1H, dd, *J*=8.6, 2.0, Ar*H*), 7.12 (1H, d, *J*=8.6, Ar*H*); δ_C (100 MHz, DMSO-d_6) 192.8 (C), 158.6 (C), 141.9 (C), 133.0 (2 x CH), 132.4 (CH), 131.6 (CH), 130.1 (2 x CH), 128.4 (C), 120.7 (C), 118.7 (C), 116.9 (CH), 114.6 (C); LCMS (APCI$^-$) 256.1 [M-H]$^-$, 100%); HRMS (FAB$^+$) Found 258.0316, $C_{14}H_9NO_2Cl$ requires 258.0322.

(4-Cyanophenyl)(3-chloro-4-hydroxyphenyl)methanol (32). A solution of $NaBH_4$ (0.59 g, 15.6 mmol) in H_2O (8 mL) was added dropwise to a solution of **31** (2.00 g, 7.75 mmol) in EtOH (25 mL). After stirring overnight, the reaction mixture was added to aq. HCl (3 M, 40 mL) and the product was extracted with DCM (3 x 30 mL). The combined organic layers were washed with brine (60 mL), dried ($MgSO_4$) and the solvent was removed *in vacuo*. The crude product was purified using Flashmaster II (EtOAc/Hexane) to give the title compound (1.45 g, 72%, mp 123-125.5 °C) as an oil which solidified on standing to give a white solid; δ_H (400 MHz, DMSO-d_6), 10.10 (1H, br s, O*H*) 7.77 (2H, AA'BB',

Ar*H*), 7.57 (2H, AA'BB', Ar*H*), 7.30 (1H, d, *J*=2.0, Ar*H*), 7.10 (1H, dd, *J*=8.4, 2.0, Ar*H*), 6.89 (1H, d, *J*=8.4, Ar*H*), 6.10 (1H, d, *J*=3.9, O*H*), 5.70 (1H, d, *J*=3.9, C*H*); δ_C (100 MHz, DMSO-d_6) 152.6 (C), 151.6 (C), 137.1 (C), 132.7 (2 x CH), 128.2 (CH), 127.4 (2 x CH), 126.6 (CH), 119.4 (C), 117.8 (C), 116.9 (CH), 109.9 (C), 73.1 (CH); LCMS (APCI$^-$) 258.0 (M^-, 100%), 240.0 (55); HRMS (FAB$^+$) Found 260.0488, $C_{14}H_{11}NO_2Cl$ requires 260.0478.

3-Bromo-4-(triisopropylsilyloxy)benzaldehyde (42). Imidazole (0.54 g, 7.94 mmol) and TIPS-Cl (0.93 g, 4.82 mmol) were sequentially added to a solution of 3-bromo-4-hydroxybenzaldehyde (0.80 g, 3.98 mmol) in DMF (8 mL). The reaction mixture was stirred overnight, then poured onto H_2O (20 ml) and extracted with EtOAc (3 x 20 ml). The combined organics were washed with H_2O (3 x 20 ml) and brine (20 ml), then dried ($MgSO_4$) and the solvent was removed *in vacuo*. The crude product was purified using Flashmaster II (EtOAc/hexane) to give the title compound as a pale yellow oil (1.34 g, 94%); δ_H (270 MHz, $CDCl_3$) 9.81 (1H, s, C*H*O), 8.05 (1H, d, *J*=1.9, Ar*H*), 7.69 (1H, dd, *J*=8.4, 1.9, Ar*H*), 6.96 (1H, d, *J*=8.4, Ar*H*), 1.41-1.10 (21H, m, 6 x CH_3, 3 x CH); LCMS (APCI$^+$) 357.4 ($[M+H]^+$, 100%).

4-((3-Bromo-4-(triisopropylsilyloxy)phenyl)(hydroxy)methyl)benzonitrile (43). ^{i}PrMgCl (2 M in THF, 12.0 mL) was slowly added to a cooled (ice/salt bath) solution of 4-iodobenzonitrile (5.05 g, 22.1 mmol) in THF (50 mL). After 30 minutes this solution was transferred by canula (over 30 minutes) to a cooled (ice/salt bath) solution of **42** (6.56 g, 18.4 mmol) in THF (100 mL). The resultant was stirred for 2 h 30 minutes with cooling and then allowed to warm to room temperature and quenched by the addition of sat. aq. NH_4Cl (50 mL) and H_2O (50 mL). The product was extracted with EtOAc (3 x 100 mL), the combined organics were washed with aq. $NaHCO_3$ (200 mL) and brine (200 mL) then dried ($MgSO_4$) and the solvent was removed in vacuo. The crude product was purified using Flashmaster II (EtOAc/Hexane) to give the title compound (6.89 g, 82%) as a colourless oil which solidified on standing; δ_H (270 MHz, $CDCl_3$) 7.62 (2H, AA'BB', Ar*H*), 7.50-7.44 (3H, m, Ar*H*), 7.06 (1H, dd, *J*=8.6, 2.2, Ar*H*), 6.83 (1H, d, *J*=8.6, Ar*H*), 5.77 (1H, d, *J*=3.1, C*H*), 2.25 (1H, d, *J*=3.1 O*H*), 1.37-1.05 (21H,

m, 6 x CH_3, 3 x CH); δ_C (100 MHz, $CDCl_3$) 152.9 (C), 148.4 (C), 136.4 (C), 132.3 (2 x CH), 131.8 (CH), 126.9 (2 x CH), 126.6 (CH), 119.6 (CH), 118.8 (C), 115.3 (C), 111.3 (C), 74.6 (CH), 17.9 (6 x CH_3), 12.9 (3 x CH); LCMS (APCI$^-$) 302.2 ([M-1)$^-$, 80%), 284.2 (100); LC/MS (APCI$^-$) 458.6 (M^--H, 10%), 390.4 (10), 302.4 (100); HRMS (ES+) calcd. for $C_{23}H_{34}BrN_2O_2Si$ (M^++NH_4) 477.1567, found 477.1563.

(4-Cyanophenyl)(3-bromo-4-hydroxyphenyl)methanol (38). TBAF (1M in THF, 12.0 mL) was added to a solution of **43** (4.55 g, 9.91 mmol) in THF (30 mL). After stirring for 15 minutes, H_2O (20 ml) was added and AcOH (3 M) was added dropwise until the solution became pale yellow. The product was extracted with EtOAc (2 x 50 ml) and the combined organic layers were washed with sat aq. $NaHCO_3$ (2 x 50 mL) and brine (50 mL) then dried ($MgSO_4$) and the solvent was removed *in vacuo*. The crude product was purified using Flashmaster II (EtOAc/Hexane) to give the title compound (2.36 g, 78 %) as previous.

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^{13}C NMR data

Bis-(3-hydroxyphenyl)methanol (**5**). δ_C (68 MHz, DMSO-d_6) 157.1 (2 x C), 147.2 (2 x C), 128.9 (2 x CH), 117.0 (2 x CH), 113.6 (2 x CH), 113.1 (2 x CH), 74.1 (CH).

1-[Bis-(3-hydroxyphenyl)methyl]-1H-[1,2,4]triazole (**6**). δ_C (100 MHz, DMSO-d_6) 158.0 (2 x C), 152.3 (CH), 144.9 (CH), 141.0 (2 x C), 130.2 (2 x CH), 119.3 (2 x CH), 115.6 (2 x CH), 115.6 (2 x CH), 66.2 (CH).

1-[Bis-(3-sulfamoyloxyphenyl)methyl]-1H-[1,2,4]triazole (**7**). δ_C (100 MHz, DMSO-d_6) 152.7 (2 x C), 150.7 (CH), 145.2 (2 x C), 140.9 (CH), 130.6 (2 x CH), 126.8 (2 x CH), 122.4 (4 x CH), 64.8 (CH)

Bis-(3-benzyloxy-4-methoxyphenyl)methanol (**13**). δ_C (100 MHz, DMSO-d_6) 149.2 (2 x C), 148.2 (2 x C), 137.2 (2 x C), 136.6 (2 x C), 128.7 (4 x CH), 128.0 (2 x CH), 127.6 (4 x CH), 119.5 (2 x CH), 112.6 (2 x CH), 111.7 (2 x CH), 75.8 (CH), 71.2 (2 x CH_2), 56.4 (2 x CH_3).

1-[Bis-(3-benzyloxy-4-methoxyphenyl)methyl]-1H-[1,2,4]triazole (**14**). δ_C (100 MHz, $CDCl_3$) 152.3 (CH), 149.9 (2 x C), 148.2 (2 x C), 143.4 (CH), 136.7 (2 x C), 130.5 (2 x C), 128.7 (4 x CH), 128.1 (2 x CH), 127.5 (4 x CH), 121.1 (2 x CH), 114.1 (2 x CH), 118.8 (2 x CH), 71.2 (2 x CH_2), 67.4 (CH), 56.4 (2 x CH_3).

1-[Bis-(3-hydroxy-4-methoxyphenyl)methyl]-1H-[1,2,4]triazole (**15**). δ_C (68 MHz, DMSO-d_6) 151.8 (CH), 147.3 (2 x C), 146.3 (2 x C), 144.0 (CH), 130.1 (2 x C), 118.8 (2 x CH), 115.3 (2 x CH), 111.9 (2 x CH), 64.9 (CH), 55.6 (2 x CH_3).

1-[Bis-(3-sulfamoyloxy-4-methoxyphenyl)methyl]-1H-[1,2,4]triazole (**16**). δ_C (68 MHz, DMSO-d_6) 151.8 (CH), 151.6 (2 x C), 144.3 (CH), 138.4 (2 x C), 131.0 (2 x C), 127.1 (2 x CH), 123.3 (2 x CH), 113.4 (2 x CH), 63.9 (CH), 56.0 (2 x CH_3).

1-[Bis-(4-hydroxy-3-methoxyphenyl)methyl]-1H-[1,2,4]triazole (**21**). δ_C (100 MHz, DMSO-d_6) 151.5 (CH), 147.4 (2 x C), 146.3 (2 x C), 144.0 (CH), 130.1 (2 x C), 120.6 (2 x CH), 115.3 (2 x CH), 112.2 (2 x CH), 65.7 (CH), 55.6 (2 x CH_3).

1-[Bis-(4-sulfamoyloxy-3-methoxyphenyl)methyl]-1H-[1,2,4]triazole (**22**). δ_C (68 MHz, DMSO-d_6) 152.1 (2 x C), 151.8 (CH), 144.6 (CH), 138.6 (2 x C), 137.8 (2 x C), 123.4 (2 x CH), 120.1 (2 x CH), 113.2 (2 x CH), 65.2 (CH), 55.9 (2 x CH_3).

1-[(4-Cyanophenyl)(4-hydroxyphenyl)methyl]-1H-[1,2,4]triazole (**27**). δ_C (100 MHz, DMSO-d_6) 158.1 (CH), 152.7 (C), 145.7 (CH), 145.0 (C), 133.2 (2 x CH), 130.4 (2 x CH), 129.2 (2 x CH), 128.7 (C), 119.2 (C), 116.2 (2 x CH), 111.2 (C), 65.4 (CH).

1-[(4-Cyanophenyl)(4-sulfamoyloxyphenyl)methyl]-1H-[1,2,4]triazole (**28**). δ_C (100 MHz, DMSO-d_6) 152.9 (CH), 150.5 (C), 145.4 (CH), 144.8 (C), 136.9 (C), 133.3 (2 x CH), 130.5 (2 x CH), 129.4 (2 x CH), 123.3 (2 x CH), 119.2 (C), 111.6 (C), 64.9 (CH).

1-[(4-Cyanophenyl)(3-chloro-4-hydroxyphenyl)methyl]-1H-[1,2,4]triazole (**33**). δ_C (100 MHz, DMSO-d_6) 153.7 (C), 152.7 (CH), 145.5 (CH), 145.0 (C), 133.1 (2 x CH), 130.4 (CH), 130.0 (C), 129.0 (2 x CH), 128.9 (CH), 120.2 (C), 119.0 (C), 117.3 (CH), 111.3 (C), 64.4 (CH).

1-[(4-Cyanophenyl)(3-chloro-4-sulfamoyloxyphenyl)methyl]-1H-[1,2,4]triazole (**34**). δ_C (100 MHz, DMSO-d_6) 152.9 (CH), 146.4 (C), 145.5 (CH), 144.1 (C), 138.1 (C), 133.3 (2 x CH), 130.8 (CH), 129.3 (2 x CH), 129.0 (CH), 127.2 (C), 124.7 (CH), 118.9 (C), 111.6 (C), 64.0 (CH).

4-Cyano-3'-bromo-4'-methoxybenzophenone (**36**). δ_C (100 MHz, DMSO-d_6) 192.0 (C), 159.2 (C), 140.9 (C), 134.1 (CH), 132.4 (2 x CH), 131.8 (CH), 129.6 (2 x CH), 129.5 (C), 118.0 (C), 114.2 (C), 112.2 (CH), 110.9 (C), 56.9 (CH_3).

4-Cyano-3'-bromo-4'-hydroxybenzophenone (**37**). δ_C (100 MHz, DMSO-d_6) 192.7 (C), 159.6 (C), 142.0 (C), 135.6 (CH), 133.2 (2 x CH), 132.4 (CH), 130.3 (2 x CH), 129.0 (C), 118.9 (C), 116.7 (CH), 114.8 (C), 110.4 (C).

(4-Cyanophenyl)(3-bromo-4-hydroxyphenyl)methanol (**38**). δ_C (100 MHz, DMSO-d_6) 154.0 (C), 151.6 (C), 137.5 (C), 132.7 (2 x CH), 131.1 (CH), 127.4 (2 x CH), 127.3 (CH), 119.4 (C), 116.6 (CH), 109.9 (C), 109.4 (C), 73.0 (CH).

1-[(4-Cyanophenyl)(3-bromo-4-hydroxyphenyl)methyl]-1H-[1,2,4]triazole (**39**). δ_C (100 MHz, DMSO-

d_6) 154.8 (C), 152.7 (CH), 145.2 (CH), 145.0 (C), 133.3 (CH), 133.1 (2 x CH), 130.4 (CH), 129.5 (CH), 129.0 (2 x CH), 119.0 (C), 116.9 (CH), 111.2 (C), 109.8 (C), 64.2 (CH).

1-[(4-Cyanophenyl)(3-bromo-4-sulfamoyloxyphenyl)methyl]-1H-[1,2,4]triazole (**40**). δ_C (100 MHz, DMSO-d_6) 152.9 (CH), 147.8 (C), 145.5 (CH), 144.1 (C), 138.2 (C), 133.8 (CH), 133.3 (2 x CH), 129.6 (CH), 129.3 (2 x CH), 124.2 (CH), 118.9 (C), 116.6 (C), 111.6 (C), 63.9 (CH).

Microanalysis data

Compound	Formula	Found %			Calculated %		
		C	H	N	C	H	N
9	$C_{15}H_{11}N_3O_2Br_2$	42.20	2.65	9.79	42.38	2.61	9.89
14	$C_{31}H_{29}N_3O_4$	73.00	5.73	8.31	73.35	5.76	8.28
15	$C_{17}H_{17}N_3O_4$	62.10	5.26	12.80	62.38	5.23	12.84
21	$C_{17}H_{17}N_3O_4$	62.45	5.23	12.80	62.38	5.23	12.84
26	$C_{14}H_{11}NO_2$	74.80	4.95	6.04	74.65	4.92	6.22
27	$C_{16}H_{12}N_4O$	69.70	4.53	19.90	69.55	4.38	20.28
39	$C_{16}H_{11}BrN_4O$	54.30	3.04	15.40	54.10	3.04	15.40

HPLC Data

Compound	HPLC Purity (>%)	R_t (min)	Solvent System
6	99	1.79	90:10 $CH_3CN:H_2O$
7	99	1.50	90:10 $CH_3CN:H_2O$
10	99	3.21	70:30 $CH_3CN:H_2O$
16	99	1.48	90:10 $CH_3CN:H_2O$
22	99	1.47	90:10 $CH_3CN:H_2O$
28	99	1.81	90:10 $CH_3CN:H_2O$
33	99	1.77	90:10 MeOH:H_2O
34	99	1.70	90:10 MeOH:H_2O
40	99	1.75	80:20 MeOH:H_2O